4-Acetamide-3-nitrophenyl acetate

Inchi: InChI=1S/C10H10N2O5/c1-6(13)11-9-4-3-8(17-7(2)14)5-10(9)12(15)16/h3-5H,1-2H3,(H,
InchiKey: HSCNPJOXRGUVFK-UHFFFAOYSA-N
Formula: C10H10N2O5
SMILES: CC(=O)Nc1ccc(OC(C)=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 238.20
CAS: 2243-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-111.43	kJ/mol	Joback Method
hf	-350.81	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	1.478		Crippen Method
mcvol	164.410	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	797.01	K	Joback Method
tc	1037.70	K	Joback Method
tf	572.28	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.62	J/mol×K	797.01	Joback Method
cpg	459.54	J/mol×K	837.13	Joback Method
cpg	468.52	J/mol×K	877.24	Joback Method
cpg	476.56	J/mol×K	917.36	Joback Method
cpg	483.70	J/mol×K	957.47	Joback Method
cpg	489.94	J/mol×K	997.59	Joback Method
cpg	495.30	J/mol×K	1037.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2243698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume